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Crystal structure of 3-(adamantan-1-yl)-4-(4-chlorophenyl)-1*H*-1,2,4-triazole-5(4*H*)-thione

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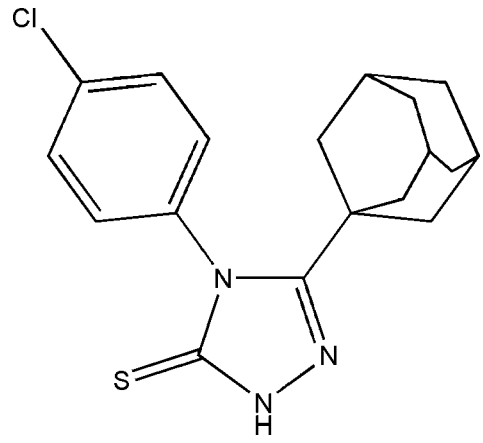
The title compound, $C_{18}H_{20}ClN_3S$, is a functionalized triazoline-3-thione derivative. The benzene ring is almost perpendicular to the planar 1,2,4-triazole ring [maximum deviation = 0.007 (1) Å] with a dihedral angle of 89.61 (5)° between them and there is an adamantane substituent at the 3-position of the triazolethione ring. In the crystal, N—H···S hydrogen-bonding interactions link the molecules into chains extending along the *c*-axis direction. The crystal packing is further stabilized by weak C—H···π interactions that link adjacent chains into a two-dimensional structure in the *bc* plane. The crystal studied was an inversion twin with a 0.50 (3):0.50 (3) domain ratio.

Keywords: crystal structure; adamantane; 1,2,4-triazole; starting material; hydrogen bonding.

CCDC reference: 1042916

1. Related literature

For the biological activity of adamantane derivatives, see: Lorenzo *et al.* (2008); Wang *et al.* (2013); Kadi *et al.* (2010); Balzarini *et al.* (2009); Protopopova *et al.* (2005); Vernier *et al.* (1969). For the biological activity of adamantyl-1,2,4-triazole derivatives, see: El-Emam & Ibrahim (1991); Al-Abdullah *et al.* (2014); El-Emam *et al.* (2004, 2013). For related adamantyl-1,2,4-triazole structures, see: El-Emam *et al.* (2012), Al-Tamimi *et al.* (2013), Al-Omary *et al.* (2014); Almutairi *et al.* (2012). For the synthesis of the title compound, see: Al-Deeb *et al.* (2006).



2. Experimental

2.1. Crystal data

$C_{18}H_{20}ClN_3S$
M_r = 345.88
Tetragonal, $I\overline{4}$
a = 23.1302 (5) Å
c = 6.4100 (2) Å
V = 3429.39 (18) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.35 mm^{-1}
T = 150 K
0.68 × 0.29 × 0.26 mm

2.2. Data collection

Bruker APEXII CCD diffractometer
106262 measured reflections
11408 independent reflections
10584 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.082
S = 1.06
11408 reflections
213 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}
Absolute structure: Flack (1983), 5353 Friedel pairs
Absolute structure parameter: 0.50 (3)

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*2 is the centroid of the C1–C6 phenyl ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H1*N*3···S1^{i}	0.92 (2)	2.46 (2)	3.3253 (9)	158.4 (19)
C13—H13*A*···*Cg*2^{ii}	0.98	2.97	3.8881 (13)	156

Symmetry codes: (i) $-x+\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (ii) $y-1, -x+1, -z+1$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2015); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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§ Thomson Reuters ResearcherID: A-3561-2009.

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Supporting information for this paper is available from the IUCr electronic archives (Reference: SJ5439).

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Crystal structure of 3-(adamantan-1-yl)-4-(4-chlorophenyl)-1*H*-1,2,4-triazole-5(4*H*)-thione

Reem I. Al-Wabli, Ali A. El-Emam, Obaid S. Alroqi, C. S. Chidan Kumar and Hoong-Kun Fun

S1. Chemical context

Adamantane derivatives have long been known for their diverse biological activities (Wang *et al.*, 2013) including anti-viral activity against influenza (Vernier *et al.*, 1969) and HIV viruses (El-Emam *et al.*, 2004; Balzarini *et al.*, 2009). In addition, adamantane derivatives are known to exhibit marked antibacterial activity (Kadi *et al.*, 2010; Protopopova *et al.*, 2005). In an earlier publication, we reported the synthesis and potent antimicrobial and anti-inflammatory activities of the title compound and its related derivatives (Al-Deeb *et al.*, 2006).

S2. Structural commentary

In the title compound (Fig. 1), the 1,2,4-triazole (N1—N3/C7/C8) ring is nearly planar with a maximum deviation of -0.007 (1) Å at atom N1. The phenyl (C1–C6) ring is almost perpendicular to the near planar 1,2,4-triazole ring with a dihedral angle of 89.61 (5) Å between them. An adamantane group is substituted at the 3-position of the triazolethione ring. The crystal studied was an inversion twin with a 0.50 (3):0.50 (3) domain ratio.

S3. Supramolecular features

In the crystal packing (Fig. 2), the molecules are linked by intermolecular N3–H1N3···S1 hydrogen bonding interactions forming chains extending along along the *c* axis direction. The crystal packing is further stabilized by weak C–H···π (phenyl) interactions (Table 1) that link the adjacent chains into a two dimensional structure in the *bc* plane.

S4. Synthesis and crystallization

The title compound was prepared by a literature procedure (Al-Deeb *et al.*, 2006) and crystallized from EtOH/$CHCl_3$ (1:1) to yield colorless crystals. M·P.: >300 °C.

^{1}H NMR ($CDCl_3$, 700.17 MHz): δ 1.55-1.70 (m, 6H, Adamantane-H), 1.86-2.05 (m, 9H, Adamantane-H), 7.25 (d, 2H, Ar—H, J = 8.5 Hz), 7.45 (d, 2H, Ar—H, J = 8.5 Hz), 11.90 (br. s, 1H, NH). 13C NMR ($CDCl_3$, 176.08 MHz): δ 27.68, 36.03, 36.44, 39.80 (Adamantane-C), 129.95, 131.02, 134.23, 136.42 (Ar—C), 158.41 (C=N), 170.0 (C=S).

S5. Refinement details

The nitrogen-bound H-atom was located in a difference Fourier map and its coordinates and isotropic displacement parameter were refined freely with d(N–H) = 0.92 (2) Å. Other H atoms were positioned geometrically (d(C–H) 0.93–0.98 Å) and refined using a riding model with U_{iso}(H) = 1.2 U_{eq}(C). The crystal studied was an inversion twin with a 0.50 (3):0.50 (3) domain ratio.

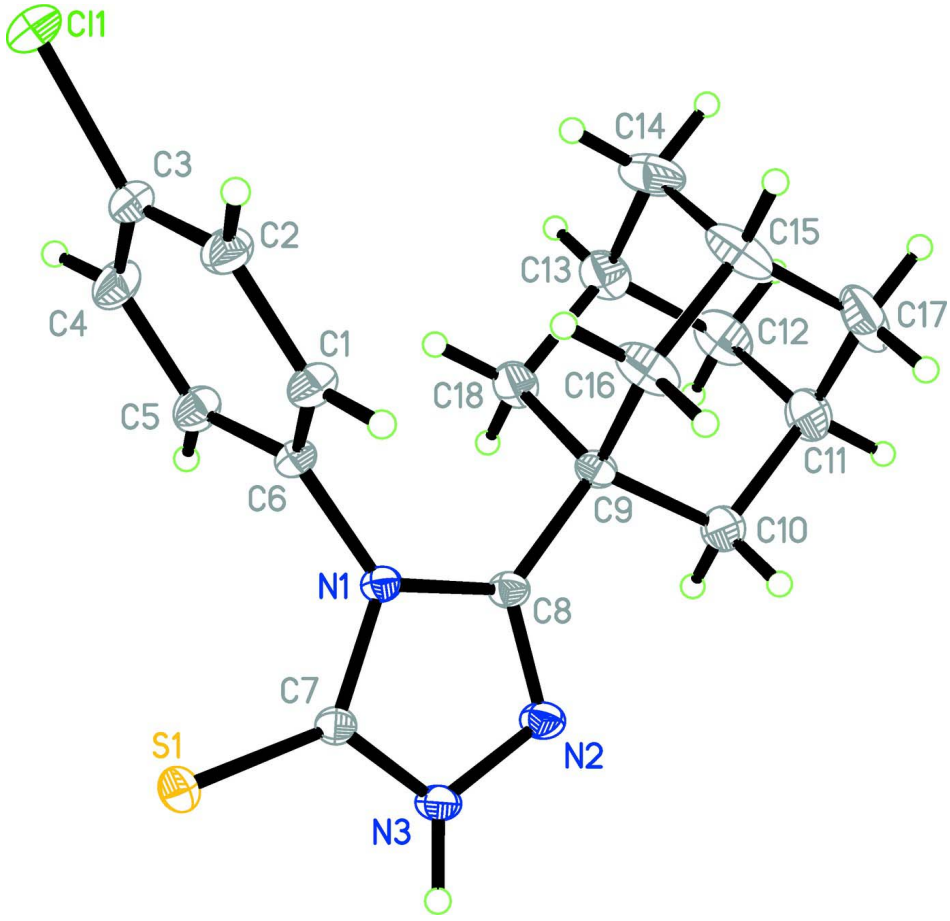

Figure 1

The molecular structure of the title compound with atom labels and 50% probability displacement ellipsoids.

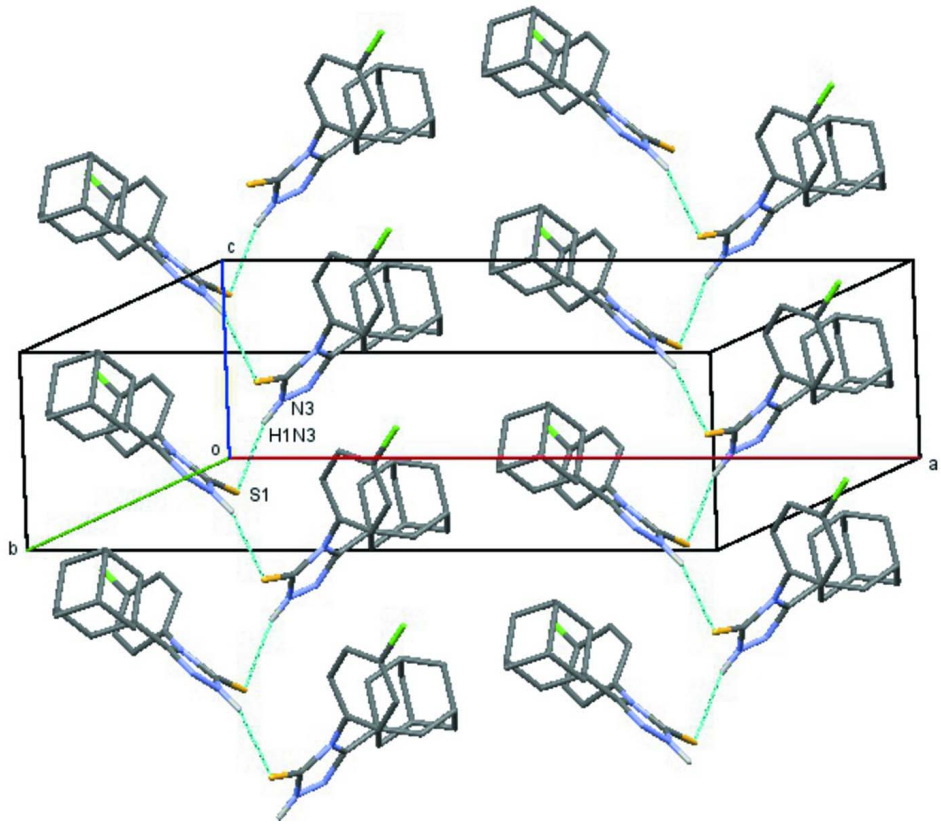

Figure 2

Crystal packing of the title compound, showing the N–H···S hydrogen bonding interactions (Table 1) as dashed lines linking the molecules into chains extending along the *c* axis direction. Other H-atoms are omited for clarity.

3-(Adamantan-1-yl)-4-(4-chlorophenyl)-1*H*-1,2,4-triazole-5(4*H*)-thione

Crystal data

$C_{18}H_{20}ClN_3S$
$M_r = 345.88$
Tetragonal, $I\bar{4}$
$a = 23.1302$ (5) Å
$c = 6.4100$ (2) Å
$V = 3429.39$ (18) Å^3
$Z = 8$
$F(000) = 1456$
$D_x = 1.340$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9155 reflections
$\theta = 2.5$–$40.8°$
$\mu = 0.35$ mm^{-1}
$T = 150$ K
Needle, colourless
0.68 × 0.29 × 0.26 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
106262 measured reflections
11408 independent reflections
10584 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 41.2°$, $\theta_{min} = 2.5°$
$h = -42 \rightarrow 42$
$k = -42 \rightarrow 42$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.082$
$S = 1.06$
11408 reflections
213 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0483P)^2 + 0.551P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.53$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}
Absolute structure: Flack (1983), 5353 Friedel pairs
Absolute structure parameter: 0.50 (3)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refined as a 2-component inversion twin.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.25120 (2)	0.81338 (2)	0.20570 (4)	0.01558 (4)
Cl1	0.10286 (2)	0.98207 (2)	0.89359 (5)	0.03118 (7)
N1	0.15119 (3)	0.77326 (3)	0.38819 (12)	0.01309 (10)
N2	0.13872 (4)	0.68822 (4)	0.23712 (14)	0.01734 (13)
N3	0.18691 (3)	0.71564 (4)	0.16208 (13)	0.01642 (12)
C1	0.16658 (4)	0.83033 (4)	0.70574 (15)	0.01686 (13)
H1A	0.1901	0.8012	0.7588	0.020*
C2	0.15555 (5)	0.87980 (4)	0.82355 (16)	0.01990 (15)
H2A	0.1715	0.8840	0.9558	0.024*
C3	0.12041 (5)	0.92258 (4)	0.74046 (17)	0.01972 (15)
C4	0.09818 (5)	0.91871 (4)	0.53962 (19)	0.02225 (17)
H4A	0.0761	0.9486	0.4843	0.027*
C5	0.10952 (4)	0.86925 (4)	0.42249 (16)	0.01916 (15)
H5A	0.0953	0.8660	0.2874	0.023*
C6	0.14220 (4)	0.82486 (4)	0.50837 (14)	0.01374 (12)
C7	0.19637 (3)	0.76715 (4)	0.25068 (13)	0.01323 (12)
C8	0.11738 (4)	0.72353 (4)	0.37613 (14)	0.01404 (12)
C9	0.06417 (3)	0.70942 (4)	0.50180 (14)	0.01456 (12)
C10	0.04492 (5)	0.64750 (5)	0.4465 (2)	0.02441 (19)
H10A	0.0368	0.6450	0.2983	0.029*
H10B	0.0758	0.6206	0.4784	0.029*
C11	−0.00943 (6)	0.63104 (5)	0.5707 (2)	0.0292 (2)
H11A	−0.0214	0.5918	0.5330	0.035*
C12	−0.05832 (5)	0.67338 (6)	0.5199 (2)	0.0292 (2)
H12A	−0.0673	0.6716	0.3722	0.035*
H12B	−0.0928	0.6628	0.5971	0.035*
C13	−0.03997 (4)	0.73459 (6)	0.5782 (2)	0.02497 (19)

H13A	−0.0715	0.7615	0.5465	0.030*
C14	−0.02609 (5)	0.73732 (7)	0.8112 (2)	0.0307 (2)
H14A	−0.0145	0.7763	0.8487	0.037*
H14B	−0.0602	0.7274	0.8916	0.037*
C15	0.02267 (5)	0.69501 (7)	0.86116 (18)	0.0303 (3)
H15A	0.0313	0.6967	1.0107	0.036*
C16	0.07706 (4)	0.71160 (6)	0.73728 (16)	0.0253 (2)
H16A	0.1082	0.6850	0.7703	0.030*
H16B	0.0893	0.7503	0.7759	0.030*
C17	0.00415 (6)	0.63344 (7)	0.8040 (3)	0.0356 (3)
H17A	0.0349	0.6065	0.8369	0.043*
H17B	−0.0298	0.6226	0.8838	0.043*
C18	0.01416 (4)	0.75172 (5)	0.45273 (18)	0.02095 (16)
H18A	0.0256	0.7908	0.4888	0.025*
H18B	0.0055	0.7507	0.3047	0.025*
H1N3	0.2084 (9)	0.6995 (9)	0.057 (4)	0.029 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01413 (8)	0.01610 (8)	0.01653 (8)	−0.00195 (6)	0.00022 (6)	0.00131 (6)
Cl1	0.04393 (16)	0.01649 (9)	0.03312 (14)	0.00301 (9)	0.01278 (12)	−0.00681 (9)
N1	0.0119 (2)	0.0135 (2)	0.0139 (3)	0.00076 (19)	0.0009 (2)	−0.0017 (2)
N2	0.0145 (3)	0.0176 (3)	0.0200 (3)	−0.0026 (2)	0.0042 (2)	−0.0047 (2)
N3	0.0140 (3)	0.0175 (3)	0.0178 (3)	−0.0019 (2)	0.0040 (2)	−0.0052 (2)
C1	0.0189 (3)	0.0158 (3)	0.0158 (3)	0.0034 (2)	−0.0032 (3)	−0.0026 (3)
C2	0.0251 (4)	0.0178 (3)	0.0168 (4)	0.0013 (3)	−0.0005 (3)	−0.0038 (3)
C3	0.0226 (4)	0.0136 (3)	0.0230 (4)	0.0011 (3)	0.0052 (3)	−0.0030 (3)
C4	0.0248 (4)	0.0151 (3)	0.0269 (5)	0.0065 (3)	−0.0008 (3)	0.0000 (3)
C5	0.0211 (4)	0.0170 (3)	0.0193 (4)	0.0048 (3)	−0.0030 (3)	0.0002 (3)
C6	0.0133 (3)	0.0127 (3)	0.0152 (3)	0.0021 (2)	0.0000 (2)	−0.0015 (2)
C7	0.0117 (3)	0.0146 (3)	0.0134 (3)	0.0007 (2)	0.0000 (2)	−0.0005 (2)
C8	0.0120 (3)	0.0152 (3)	0.0149 (3)	0.0001 (2)	0.0010 (2)	−0.0016 (2)
C9	0.0113 (3)	0.0177 (3)	0.0146 (3)	−0.0002 (2)	0.0011 (2)	0.0002 (3)
C10	0.0227 (4)	0.0184 (4)	0.0322 (5)	−0.0046 (3)	0.0090 (4)	−0.0016 (3)
C11	0.0251 (5)	0.0242 (4)	0.0382 (6)	−0.0082 (4)	0.0103 (4)	0.0016 (4)
C12	0.0150 (4)	0.0438 (6)	0.0288 (5)	−0.0089 (4)	−0.0016 (3)	0.0016 (5)
C13	0.0125 (3)	0.0319 (5)	0.0305 (5)	0.0038 (3)	0.0031 (3)	0.0058 (4)
C14	0.0208 (4)	0.0435 (7)	0.0280 (5)	−0.0009 (4)	0.0101 (4)	−0.0069 (5)
C15	0.0181 (4)	0.0568 (8)	0.0161 (4)	−0.0046 (4)	0.0023 (3)	0.0064 (4)
C16	0.0140 (3)	0.0462 (6)	0.0157 (4)	−0.0035 (4)	−0.0010 (3)	0.0036 (4)
C17	0.0241 (5)	0.0438 (7)	0.0388 (7)	0.0009 (5)	0.0085 (5)	0.0235 (6)
C18	0.0134 (3)	0.0238 (4)	0.0256 (4)	0.0034 (3)	0.0018 (3)	0.0055 (3)

Geometric parameters (Å, º)

S1—C7	1.6836 (9)	C10—H10A	0.9700
Cl1—C3	1.7384 (10)	C10—H10B	0.9700

N1—C7	1.3744 (11)	C11—C17	1.529 (2)
N1—C8	1.3931 (11)	C11—C12	1.531 (2)
N1—C6	1.4355 (11)	C11—H11A	0.9800
N2—C8	1.3056 (12)	C12—C13	1.5246 (19)
N2—N3	1.3696 (11)	C12—H12A	0.9700
N3—C7	1.3379 (12)	C12—H12B	0.9700
N3—H1N3	0.92 (2)	C13—C14	1.529 (2)
C1—C6	1.3909 (13)	C13—C18	1.5399 (15)
C1—C2	1.3946 (13)	C13—H13A	0.9800
C1—H1A	0.9300	C14—C15	1.527 (2)
C2—C3	1.3869 (14)	C14—H14A	0.9700
C2—H2A	0.9300	C14—H14B	0.9700
C3—C4	1.3892 (16)	C15—C17	1.532 (2)
C4—C5	1.3933 (14)	C15—C16	1.5362 (15)
C4—H4A	0.9300	C15—H15A	0.9800
C5—C6	1.3889 (12)	C16—H16A	0.9700
C5—H5A	0.9300	C16—H16B	0.9700
C8—C9	1.5067 (12)	C17—H17A	0.9700
C9—C16	1.5394 (14)	C17—H17B	0.9700
C9—C10	1.5413 (14)	C18—H18A	0.9700
C9—C18	1.5473 (13)	C18—H18B	0.9700
C10—C11	1.5359 (15)		

C7—N1—C8	107.83 (7)	C17—C11—H11A	109.4
C7—N1—C6	122.67 (7)	C12—C11—H11A	109.4
C8—N1—C6	129.42 (7)	C10—C11—H11A	109.4
C8—N2—N3	104.93 (7)	C13—C12—C11	109.64 (9)
C7—N3—N2	113.35 (7)	C13—C12—H12A	109.7
C7—N3—H1N3	125.9 (14)	C11—C12—H12A	109.7
N2—N3—H1N3	120.7 (14)	C13—C12—H12B	109.7
C6—C1—C2	119.54 (8)	C11—C12—H12B	109.7
C6—C1—H1A	120.2	H12A—C12—H12B	108.2
C2—C1—H1A	120.2	C12—C13—C14	109.65 (11)
C3—C2—C1	118.99 (9)	C12—C13—C18	109.72 (10)
C3—C2—H2A	120.5	C14—C13—C18	109.20 (9)
C1—C2—H2A	120.5	C12—C13—H13A	109.4
C2—C3—C4	121.80 (9)	C14—C13—H13A	109.4
C2—C3—Cl1	119.00 (8)	C18—C13—H13A	109.4
C4—C3—Cl1	119.20 (8)	C15—C14—C13	109.46 (10)
C3—C4—C5	118.85 (9)	C15—C14—H14A	109.8
C3—C4—H4A	120.6	C13—C14—H14A	109.8
C5—C4—H4A	120.6	C15—C14—H14B	109.8
C6—C5—C4	119.73 (9)	C13—C14—H14B	109.8
C6—C5—H5A	120.1	H14A—C14—H14B	108.2
C4—C5—H5A	120.1	C14—C15—C17	109.82 (10)
C5—C6—C1	120.93 (8)	C14—C15—C16	109.66 (11)
C5—C6—N1	118.74 (8)	C17—C15—C16	109.74 (11)
C1—C6—N1	120.33 (7)	C14—C15—H15A	109.2

N3—C7—N1	103.86 (7)	C17—C15—H15A	109.2
N3—C7—S1	128.03 (7)	C16—C15—H15A	109.2
N1—C7—S1	128.11 (7)	C15—C16—C9	109.88 (8)
N2—C8—N1	110.01 (8)	C15—C16—H16A	109.7
N2—C8—C9	122.57 (8)	C9—C16—H16A	109.7
N1—C8—C9	127.42 (8)	C15—C16—H16B	109.7
C8—C9—C16	111.04 (7)	C9—C16—H16B	109.7
C8—C9—C10	108.32 (7)	H16A—C16—H16B	108.2
C16—C9—C10	108.17 (9)	C11—C17—C15	108.97 (10)
C8—C9—C18	111.41 (8)	C11—C17—H17A	109.9
C16—C9—C18	108.87 (8)	C15—C17—H17A	109.9
C10—C9—C18	108.96 (8)	C11—C17—H17B	109.9
C11—C10—C9	110.34 (9)	C15—C17—H17B	109.9
C11—C10—H10A	109.6	H17A—C17—H17B	108.3
C9—C10—H10A	109.6	C13—C18—C9	109.81 (8)
C11—C10—H10B	109.6	C13—C18—H18A	109.7
C9—C10—H10B	109.6	C9—C18—H18A	109.7
H10A—C10—H10B	108.1	C13—C18—H18B	109.7
C17—C11—C12	109.66 (11)	C9—C18—H18B	109.7
C17—C11—C10	109.25 (11)	H18A—C18—H18B	108.2
C12—C11—C10	109.63 (10)		

C8—N2—N3—C7	0.12 (11)	N1—C8—C9—C10	−175.22 (9)
C6—C1—C2—C3	−0.08 (15)	N2—C8—C9—C18	−115.92 (10)
C1—C2—C3—C4	−3.09 (16)	N1—C8—C9—C18	64.95 (12)
C1—C2—C3—Cl1	175.90 (8)	C8—C9—C10—C11	−179.89 (10)
C2—C3—C4—C5	2.89 (17)	C16—C9—C10—C11	59.67 (12)
Cl1—C3—C4—C5	−176.10 (9)	C18—C9—C10—C11	−58.54 (13)
C3—C4—C5—C6	0.48 (16)	C9—C10—C11—C17	−60.75 (14)
C4—C5—C6—C1	−3.62 (15)	C9—C10—C11—C12	59.44 (14)
C4—C5—C6—N1	177.30 (9)	C17—C11—C12—C13	59.98 (13)
C2—C1—C6—C5	3.41 (14)	C10—C11—C12—C13	−59.96 (14)
C2—C1—C6—N1	−177.52 (9)	C11—C12—C13—C14	−59.57 (12)
C7—N1—C6—C5	88.15 (11)	C11—C12—C13—C18	60.37 (13)
C8—N1—C6—C5	−88.12 (12)	C12—C13—C14—C15	59.55 (12)
C7—N1—C6—C1	−90.93 (11)	C18—C13—C14—C15	−60.70 (14)
C8—N1—C6—C1	92.80 (11)	C13—C14—C15—C17	−59.99 (13)
N2—N3—C7—N1	−0.81 (10)	C13—C14—C15—C16	60.67 (14)
N2—N3—C7—S1	178.68 (7)	C14—C15—C16—C9	−60.06 (15)
C8—N1—C7—N3	1.15 (9)	C17—C15—C16—C9	60.65 (14)
C6—N1—C7—N3	−175.82 (8)	C8—C9—C16—C15	−178.05 (10)
C8—N1—C7—S1	−178.34 (7)	C10—C9—C16—C15	−59.33 (13)
C6—N1—C7—S1	4.69 (12)	C18—C9—C16—C15	58.94 (13)
N3—N2—C8—N1	0.64 (10)	C12—C11—C17—C15	−59.90 (12)
N3—N2—C8—C9	−178.62 (8)	C10—C11—C17—C15	60.27 (13)
C7—N1—C8—N2	−1.17 (10)	C14—C15—C17—C11	60.10 (13)
C6—N1—C8—N2	175.53 (9)	C16—C15—C17—C11	−60.52 (13)
C7—N1—C8—C9	178.05 (8)	C12—C13—C18—C9	−59.95 (12)

C6—N1—C8—C9	−5.25 (15)	C14—C13—C18—C9	60.26 (13)
N2—C8—C9—C16	122.54 (11)	C8—C9—C18—C13	178.01 (9)
N1—C8—C9—C16	−56.58 (13)	C16—C9—C18—C13	−59.20 (12)
N2—C8—C9—C10	3.91 (13)	C10—C9—C18—C13	58.56 (12)

Hydrogen-bond geometry (Å, º)

Cg2 is the centroid of the C1–C6 phenyl ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H1*N*3···S1^{i}	0.92 (2)	2.46 (2)	3.3253 (9)	158.4 (19)
C13—H13*A*···*Cg*2^{ii}	0.98	2.97	3.8881 (13)	156

Symmetry codes: (i) −*x*+1/2, −*y*+3/2, *z*−1/2; (ii) *y*−1, −*x*+1, −*z*+1.